PENGARUH PENAMBAHAN LAPISAN rGO TERHADAP ENERGI ADSORPSI DAN BANDGAP Sr-LaFeO_3 SEBAGAI SENSOR GAS ETANOL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY*

SKRIPSI

diajukan untuk memenuhi salah satu syarat memperoleh gelar Sarjana Sains

Program Studi Fisika Kelompok Bidang Kajian Fisika Material

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PROGRAM STUDI FISIKA

FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM

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Oleh

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Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat memperoleh gelar
Sarjana Sains pada Program Studi Fisika
Konsentrasi Fisika Material
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PERNYATAAN

Dengan ini saya menyatakan bahwa skripsi dengan judul “PENGARUH PENAMBAHAN LAPISAN rGO TERHADAP ENERGI ADSORPSI DAN BANDGAP Sr-$LaFeO_3$ SEBAGAI SENSOR GAS ETANOL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY*” ini beserta seluruh isinya adalah benar-benar karya saya sendiri. Saya tidak melakukan penjiplakan atau pengutipan dengan cara-cara yang tidak sesuai dengan etika ilmu yang berlaku dalam masyarakat keilmuan. Atas pernyataan ini, saya siap menanggung risiko/sanksi apabila di kemudian hari ditemukan adanya pelanggaran etika keilmuan atau ada klaim dari pihak lain terhadap keaslian karya saya ini.

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ABSTRAK

Material $LaFeO_3$ atau *Lanthanum orthoferrite* merupakan material yang berpotensi sebagai bahan pembuat sensor gas yang molekul gas penyusunnya terdiri dari oksigen. Namun, $LaFeO_3$ sebagai bahan sensor gas etanol memiliki kinerja yang kurang optimal dalam hal sensitivitas dan selektivitas sehingga diperlukan pemberian *doping*. *Doping* Strontium (Sr) dipilih untuk meningkatkan sensitivitas sensor gas. Selain itu, penambahan lapisan *reduce graphene oxide* (rGO) dapat meningkatkan selektivitas sensor gas etanol. Penelitian ini bertujuan untuk mempelajari pengaruh penambahan lapisan rGO terhadap energi adsorpsi dan *bandgap* $SrLaFeO_3$ (SLFO) sebagai sensor gas etanol menggunakan *Density Functional Theory* (DFT). Perhitungan DFT dilakukan untuk menghitung energi adsorpsi dan energi *bandgap* $SrLaFeO_3$ murni dan $SrLaFeO_3$ dengan penambahan lapisan rGO ketika mendapat paparan molekul etanol. Pada penelitian ini, energi adsorpsi $SrLaFeO_3$ ketika terpapar etanol bernilai -5,12 eV dan menjadi -6,09 eV setelah diberi lapisan rGO sedangkan untuk energi *bandgap* $SrLaFeO_3$ murni sebesar 0,83 eV dan ketika dilapisi rGO menjadi 0,04 eV. Untuk $SrLaFeO_3$ yang terpapar etanol bernilai 0,40 eV dan menjadi 0,02 eV ketika dilapisi rGO. Berdasarkan hasil tersebut penambahan lapisan rGO dapat memperkecil energi *bandgap* $SrLaFeO_3$ dan berpotensi dapat meningkatkan sensitivitas dan selektivitas sensor gas etanol berbasis $SrLaFeO_3$.

Kata kunci: $LaFeO_3$, Strontium, $SrLaFeO_3$, *reduce graphene oxide*, sensor gas etanol, *density functional theory*

ABSTRACT

$LaFeO_3$ or Lanthanum orthoferrite material is a potential material as a component of a gas sensor whose gas molecules consist of oxygen. However, $LaFeO_3$ as an ethanol gas sensor material has less than optimal performance in terms of sensitivity and selectivity so that doping is required. Strontium (Sr) doping was chosen to increase the sensitivity of the gas sensor. In addition, the addition of a reduced graphene oxide (rGO) layer can increase the selectivity of the ethanol gas sensor. This study aims to study the effect of adding an rGO layer on the adsorption energy and bandgap energy of $SrLaFeO_3$ (SLFO) as an ethanol gas sensor using Density Functional Theory (DFT). DFT calculations were carried out to calculate the adsorption energy and bandgap energy of pure $SrLaFeO_3$ and $SrLaFeO_3$ with the addition of an rGO layer to exposure to ethanol molecules. In this study, the adsorption energy of $SrLaFeO_3$ when exposed to ethanol was -5.12 eV and became -6.09 eV after being coated with rGO. For $SrLaFeO_3$ bandgap energy is 0,83 eV and when coated with rGO becomes 0.04 eV. For $SrLaFeO_3$ exposed to ethanol is 0.40 eV and becomes 0.02 eV when coated with rGO. Based on these results, the addition of rGO layer can reduce the bandgap energy of $SrLaFeO_3$ and has the potential to increase the sensitivity and selectivity of $SrLaFeO_3$-based ethanol gas sensors.

Keywords: $LaFeO_3$, Strontium, $SrLaFeO_3$, reduce graphene oxide, ethanol gas sensor, density functional theory

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